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3-Phenyl-1,5-di-2-pyridylpentane-1,5-dione

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.141
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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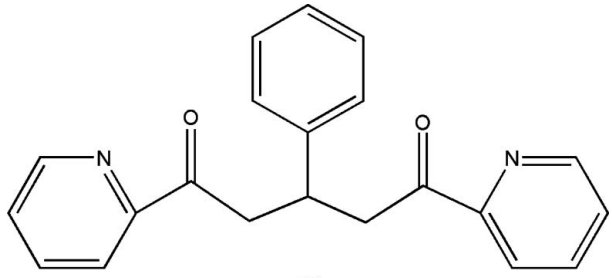
In the title compound, $C_{21}H_{18}N_2O_2$, synthesized by the reaction of benzaldehyde with 2-acetylpyridine and KOH, the phenyl ring makes dihedral angles of 88.5 (1) and 83.9 (1)° with the two pyridine rings. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds, with an H···O distance of 2.47 Å, and by van der Waals forces.

Comment

In continuation of our ongoing programme directed towards the development of environmentally benign methods of chemical synthesis (Hajipour *et al.*, 2004, 2005), we have discovered a convenient one-step method for the preparation of 1,5-diketones, starting from fragrant aldehydes and fragrant ketones, in the presence of KOH under solvent-free conditions. Using this method, which can be considered as a a general method for the synthesis of 1,5-diketones, we obtained the title compound, (I). We present here its crystal structure.



(I)

In (I) (Fig. 1), the bond lengths and angles are normal (Allen *et al.*, 1987). The phenyl ring makes dihedral angles of 88.5 (1) and 83.9 (1)° with pyridine rings N1/C6/C8–C11 and N2/C18/C20–23, respectively. Weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Interestingly, the molecular geometry, the topology of the crystal packing and the triclinic unit-cell parameters of (I) are close to those observed for 3-(4-fluorophenyl)pentane-1,5-di-2-pyridyl-1,5-dione (Constable *et al.*, 1998).

Experimental

2-Acetylpyridine (0.76 g, 6.25 mmol), freshly distilled benzaldehyde (0.33 g, 3.125 mmol) and KOH (0.35 g, 6.25 mmol) were mixed with a glass paddle in an open flask. The resulting mixture was washed with water several times to remove the KOH and recrystallized from ethanol, affording the title compound as a crystalline solid.

Crystal data

$C_{21}H_{18}N_2O_2$
$M_r = 330.37$
Triclinic, $P\overline{1}$
$a = 8.464$ (3) Å
$b = 10.484$ (4) Å
$c = 10.713$ (4) Å
$\alpha = 94.449$ (4)°
$\beta = 111.377$ (4)°
$\gamma = 100.396$ (4)°
$V = 860.0$ (5) Å^3
$Z = 2$
$D_x = 1.276$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.56 × 0.53 × 0.48 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.955$, $T_{max} = 0.961$
4446 measured reflections
2983 independent reflections
2152 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.141$
$S = 1.00$
2983 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 0.1387P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O2^{i}	0.93	2.47	3.289 (3)	147

Symmetry code: (i) $-x+1, -y, -z+2$.

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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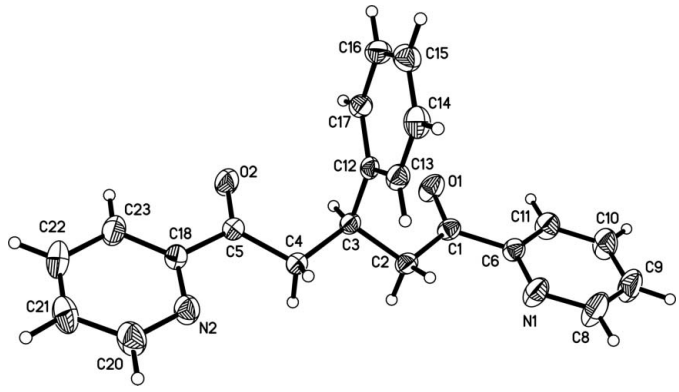

Figure 1
The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 30% probability level.

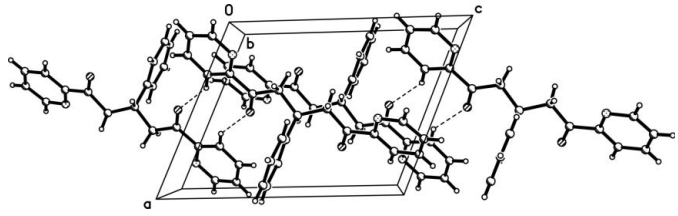

Figure 2
The packing of (I), viewed along the *b* axis. Dashed lines denote C—H···O hydrogen bonds.

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